Semiclassical approximations for adiabatic slow-fast systems

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Abstract

In this letter we give a systematic derivation and justification of the semiclassical model for the slow degrees of freedom in adiabatic slow-fast systems first found by Littlejohn and Flynn [5]. The classical Hamiltonian obtains a correction due to the variation of the adiabatic subspaces and the symplectic form is modified by the curvature of the Berry connection. We show that this classical system can be used to approximate quantum mechanical expectations and the time-evolution of operators also in sub-leading order in the combined adiabatic and semiclassical limit. In solid state physics the corresponding semiclassical description of Bloch electrons has led to substantial progress during the recent years, see [1]. Here, as an illustration, we show how to compute the Piezo-current arising from a slow deformation of a crystal in the presence of a constant magnetic field.

Consider a quantum system with a Hamiltonian $\hat{H} = H(x, -\mathrm{i}\varepsilon\nabla_x)$ given by the Weyl quantization of an operator valued symbol $H(q,p)$ acting on a Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n_x) \otimes \mathcal{H}_\mathrm{f} \cong L^2(\mathbb{R}^n_x, \mathcal{H}_\mathrm{f})$. Systems composed of *slow* degrees of freedom with configuration space $\mathbb{R}^n_x$ and *fast* degrees of freedom with state space $\mathcal{H}_\mathrm{f}$ are of this form. The small dimensionless parameter $\varepsilon \ll 1$ controls the separation of time scales and the limit $\varepsilon \to 0$ corresponds to an adiabatic limit, in which the slow and fast degrees of freedom decouple. At the same time $\varepsilon \to 0$ is the semiclassical limit for the slow degrees of freedom. Concrete realizations of this setting are the Born-Oppenheimer approximation [2], the semiclassical limit of particles with spin [3], Bloch electrons in weak fields [11] and many others, see also [4] and references therein.

In this letter we show that with each isolated eigenvalue $e(q,p)$ of the symbol $H(q,p)$ there is associated a classical system with an ε-dependent Hamilton function $h(q,p) = e(q,p) + \varepsilon M(q,p)$ and a modified symplectic form $\omega(q,p) = \omega_0 + \varepsilon\Omega(q,p)$. Here M and Ω depend also on the corresponding spectral projection $\pi_0(q,p)$ of $H(q,p)$. The correction to the energy M results from a super-adiabatic approximation: the true state of the fast degrees of freedom is in the range of a slight modification $\hat{\pi}$ of the adiabatic projector $\hat{\pi}_0 = \pi_0(x, -\mathrm{i}\varepsilon\nabla_x)$. The correction Ω to the symplectic form is given by the curvature of the Berry connection and takes into account the geometry of the eigenspace bundle defined by $\pi_0(q,p)$. We show that with the help of this classical system one can approximate expectations for "slow" observables $\hat{a} \otimes \mathbf{1}_{\mathcal{H}_\mathrm{f}}$ and also their time-evolution in the Heisenberg picture with errors of order $\mathcal{O}(\varepsilon^2)$.

The classical system described above appeared first in the seminal work of Littlejohn and Flynn [5] in the context of WKB approximations. But they neither claimed nor proved the statements of the present paper. Independently, Niu and coworkers [1] applied the classical model with

enormous success in the context of the semiclassical description of Bloch electrons. Here the classical description provides simple and straightforward derivations of formulas that are hard to justify by other means.

Given the abundance of slow-fast systems in physics, a complete understanding of their semiclassical limit is desirable. The main novelty presented in this letter are general and systematic proofs showing that the classical model indeed approximates the quantum mechanical expectations of time-dependent "slow" observables. Our approach differs from earlier ones in two ways. Based on [6], it is intrinsically gauge invariant as it does not use a local choice of eigenfunctions for the fast system. And it directly applies to arbitrary states, not only to semiclassical wave packets. For a mathematically rigorous formulation of our results we refer to [7].

The structure of this letter is as follows. We first recall a few basic facts about the Weyl calculus and the adiabatic approximation. Then we construct the classical Hamiltonian system and prove the various semiclassical approximations. Finally we show how to incorporate also time-dependent Hamiltonians and compute, as an illustration, the Piezo-current in the presence of a magnetic field. We conclude with some remarks on the literature.

1 Preliminaries and definitions

1.1 Weyl calculus

With a function $A : \mathbb{R}^{2n} \to \mathcal{L}(\mathcal{H}_\mathrm{f})$ on classical phase space taking values in the linear operators on $\mathcal{H}_\mathrm{f}$ one associates the Weyl operator

$$(\hat{A}\psi)(x) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^{2n}} \mathrm{d}p\mathrm{d}y A\left(\tfrac{1}{2}(x+y), p\right) \mathrm{e}^{\mathrm{i}p\cdot(x-y)/\varepsilon} \psi(y)$$

acting on $\psi \in \mathcal{H} = L^2(\mathbb{R}^n_x, \mathcal{H}_\mathrm{f})$. The composition of operators $\hat{A}\hat{B} = \hat{C}$ induces a composition of symbols denoted by $C = A\#B$ and called the Moyal product. The asymptotic expansion of $A\#B$ starts with

$$A\#B \asymp A_0B_0 + \varepsilon(A_1B_0 + A_0B_1 - \tfrac{\mathrm{i}}{2}\{A_0, B_0\}) + \mathcal{O}(\varepsilon^2),$$

where $\{\cdot,\cdot\}$ denotes the Poisson bracket $\{A_0, B_0\} = \sum_{j=1}^n \left(\partial_{p_j}A_0\,\partial_{q_j}B_0 - \partial_{q_j}A_0\,\partial_{p_j}B_0\right)$. Since A_0 and B_0 are operator valued functions, they do not commute in general and neither do their derivatives. Hence, in general, $\{A, A\} \neq 0$, but, if the derivatives of A are trace-class,

$$\mathrm{tr}\left(\{A, A\}\right) = 0\,, \tag{1}$$

because of the cyclicity of the trace. For later reference we state also the subprincipal symbol for triple products

$$\begin{aligned}(A\#B\#C)_1 = {} & A_1B_0C_0 + A_0B_1C_0 + A_0B_0C_1 \\ & -\tfrac{\mathrm{i}}{2}(A_0\{B_0, C_0\} + \{A_0, B_0\}C_0 + \{A_0|B_0|C_0\})\,.\end{aligned} \tag{2}$$

Here and in the following we use the shorthand

$$\{A_0|B_0|C_0\} \;:=\; \partial_pA_0\cdot B_0\,\partial_qC_0 - \partial_qA_0\cdot B_0\,\partial_pC_0\,.$$

If a symbol $A = a \cdot \mathrm{id}$ is a scalar multiple of the identity, then A and all its derivatives commute with any B. As a consequence one can show that in this case

$$A_0 \# B_0 - B_0 \# A_0 \asymp -\mathrm{i}\varepsilon\{A_0, B_0\} + \mathcal{O}(\varepsilon^3)\,. \tag{3}$$

The fact that the remainder term in (3) is of order ε^3 and not only ε^2 is at the basis of higher order semiclassical approximations. Note that $\pi_0^2 = \pi_0$ implies that any partial derivative $\partial_j \pi_0$ is off-diagonal with respect to π_0,

$$\partial_j \pi_0 = \pi_0 (\partial_j \pi_0) \pi_0^{\perp} + \pi_0^{\perp} (\partial_j \pi_0) \pi_0\,, \tag{4}$$

with $\pi_0^{\perp} = 1 - \pi_0$. Thus for scalar symbols $a = a \mathbf{1}_{\mathcal{H}_\mathrm{f}}$

$$\{a, \pi_0\} = \pi_0 \{a, \pi_0\} \pi_0^{\perp} + \pi_0^{\perp} \{a, \pi_0\} \pi_0. \tag{5}$$

Finally one can express the trace of a product of Weyl operators by a classical phase space integral,

$$\mathrm{Tr}\big(\hat{A}\hat{B}\big) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^{2n}} \mathrm{d}q \mathrm{d}p \; \mathrm{tr}(A(q,p)B(q,p))\,. \tag{6}$$

Here Tr denotes the trace on $\mathcal{H}$ and tr the trace on $\mathcal{H}_\mathrm{f}$.

1.2 Adiabatic approximation

Let $e_0(q,p)$ be a non-degenerate eigenvalue band of the principal symbol $H_0(q,p)$ of the Hamiltonian $\hat{H} = \hat{H}_0 + \varepsilon \hat{H}_1$ and $\pi_0(q,p)$ the corresponding family of rank one spectral projections. Then there exists an associated subspace $\hat{\pi}\mathcal{H}$ of $\mathcal{H}$ that is adiabatically invariant:

Claim: There exists a projection $\hat{\pi}$ with symbol $\pi = \pi_0 + \varepsilon \pi_1 + \mathcal{O}(\varepsilon^2)$ such that $[\hat{\pi}, \hat{H}] = \mathcal{O}(\varepsilon^\infty)$. As a consequence, the range of $\hat{\pi}$ is almost invariant, $[\hat{\pi}, \mathrm{e}^{-\mathrm{i}\hat{H}\frac{t}{\varepsilon}}] = \mathcal{O}(\varepsilon^\infty |t|)$, and the adiabatic approximation $\mathrm{e}^{-\mathrm{i}\hat{H}\frac{t}{\varepsilon}}\hat{\pi} = \mathrm{e}^{-\mathrm{i}\hat{\pi}\hat{H}\hat{\pi}\frac{t}{\varepsilon}}\hat{\pi} + \mathcal{O}(\varepsilon^\infty|t|)$ holds. Moreover

$$\pi_0 \pi_1 \pi_0 = \tfrac{\mathrm{i}}{2}\, \pi_0 \{\pi_0, \pi_0\} \pi_0\,. \tag{7}$$

Proof. The construction of π was first done in [6] and is by now standard, c.f. [4]. Equation (7) simply follows from the fact that π is a projector in the Moyal algebra, $0 = \pi \# \pi - \pi = \varepsilon(\pi_1 \pi_0 + \pi_0 \pi_1 - \frac{\mathrm{i}}{2}\{\pi_0, \pi_0\} - \pi_1) + \mathcal{O}(\varepsilon^2)$.

1.3 The classical Hamiltonian

It therefore suffices to study the restriction $\hat{\pi}\hat{H}\hat{\pi}$ of $\hat{H}$ to the adiabatic subspace $\hat{\pi}\mathcal{H}$ in order to understand the dynamics within $\hat{\pi}\mathcal{H}$. We will show that its semiclassical limit is governed by the associated scalar Hamilton function

$$h := e + \varepsilon M,$$

with $e = e_0 + \varepsilon \mathrm{tr}(H_1 \pi_0)$ and $M := \frac{\mathrm{i}}{2}\,\mathrm{tr}\,(\{\pi_0 | H_0 | \pi_0\})$.

Claim: It holds that $\pi \# h \# \pi - \pi \# H \# \pi = \mathcal{O}(\varepsilon^2)$ and thus $\hat{\pi}\,\hat{h}\,\hat{\pi} - \hat{\pi}\,\hat{H}\,\hat{\pi} = \mathcal{O}(\varepsilon^2)$.

Proof: In the expansion of $\pi \# h \# \pi - \pi \# H \# \pi$ the principal symbol vanishes and the subprincipal

symbol is $M\pi_0 + \frac{\mathrm{i}}{2}(\pi_0\{H_0 - e_0, \pi_0\} + \{\pi_0, H_0 - e_0\}\pi_0 + \{\pi_0|H_0 - e_0|\pi_0\})$. To see that it also vanishes, note that (1) and (4) imply

$$\begin{aligned} M\pi_0 &= \tfrac{\mathrm{i}}{2}\mathrm{tr}\left(\{\pi_0|H_0|\pi_0\}\right)\pi_0 \overset{(1)}{=} \tfrac{\mathrm{i}}{2}\mathrm{tr}\left(\{\pi_0|H_0 - e_0|\pi_0\}\right)\pi_0 \\ &\overset{(4)}{=} \tfrac{\mathrm{i}}{2}\mathrm{tr}\left(\pi_0\{\pi_0|H_0 - e_0|\pi_0\}\pi_0\right)\pi_0 \\ &= \tfrac{\mathrm{i}}{2}\pi_0\{\pi_0|H_0 - e_0|\pi_0\}\pi_0 \overset{(4)}{=} \tfrac{\mathrm{i}}{2}\{\pi_0|H_0 - e_0|\pi_0\}\,. \end{aligned}$$

Moreover $0 = \partial_j\big((H_0 - e_0)\pi_0\big)\pi_0 = \partial_j(H_0 - e_0)\pi_0 + (H_0 - e_0)\partial_j\pi_0\pi_0$ implies that $-\{\pi_0, H_0 - e_0\}\pi_0 = \{\pi_0|H_0 - e_0|\pi_0\}\pi_0 = \{\pi_0|H_0 - e_0|\pi_0\}$, which proves the claim and shows also $M = \frac{\mathrm{i}}{2}\mathrm{tr}\left(\{\pi_0|H_0 - e_0|\pi_0\}\right) = -\frac{\mathrm{i}}{2}\mathrm{tr}\left(\pi_0\{\pi_0, H_0 - e_0\}\right)$.

1.4 The symplectic form and its Liouville measure

In order to obtain semiclassical approximations up to errors of order ε^2, one needs to take into account that the restriction to the range of $\hat\pi$ also induces a modified symplectic form ω_ε on $\mathbb{R}^{2n}$ given by

$$\omega_\varepsilon := \omega_0 + \varepsilon\,\Omega = \begin{pmatrix} 0 & E_n \\ -E_n & 0 \end{pmatrix} \,+\, \varepsilon \begin{pmatrix} \Omega^{qq} & \Omega^{qp} \\ \Omega^{pq} & \Omega^{pp} \end{pmatrix},$$

where the components of Ω in the canonical basis are

$$\Omega_{\alpha\beta} \;:=\; -\,\mathrm{i}\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(\pi_0[\partial_{z_\alpha}\pi_0, \partial_{z_\beta}\pi_0]\right)\,,$$

with $z = (q,p)$ and $\alpha, \beta = 1, \ldots, 2n$. By definition Ω is skew-symmetric and one readily checks that it defines a closed 2-form. Actually Ω is the curvature 2-form of the Berry connection. For ε small enough ω_ε is thus a symplectic form. The Liouville measure λ_ε associated with the symplectic form ω_ε has the expansion

$$\begin{aligned} \lambda_\varepsilon &= \Big(1 + \tfrac{\varepsilon}{2}\sum_{j=1}^{n}\left(\Omega^{qp}_{jj} - \Omega^{pq}_{jj}\right)\Big)\mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n + \mathcal{O}(\varepsilon^2) \\ &= \left(1 + \mathrm{i}\varepsilon\,\mathrm{tr}\left(\pi_0\{\pi_0, \pi_0\}\right)\right)\mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}p^n + \mathcal{O}(\varepsilon^2). \end{aligned}$$

2 Results: Semiclassical approximations

2.1 Equilibrium expectations

Let $a : \mathbb{R}^{2n} \to \mathbb{R}$ be integrable and $f : \mathbb{R} \to \mathbb{R}$ be smooth, then

$$\mathrm{Tr}\left(\hat\pi f(\hat H)\,\hat a\right) = \frac{1}{(2\pi\varepsilon)^n}\int \mathrm{d}\lambda_\varepsilon\; f(h(q,p))\,a(q,p) + \mathcal{O}(\varepsilon^{2-n}). \tag{8}$$

Proof: In the following computation we use that $[\hat\pi, \hat H] = \mathcal{O}(\varepsilon^\infty)$ and $[\hat\pi, \hat h] = \mathcal{O}(\varepsilon)$ imply also $[\hat\pi, f(\hat H)] = \mathcal{O}(\varepsilon^\infty)$ and $[\hat\pi, f(\hat h)] = \mathcal{O}(\varepsilon)$, and, $\hat\pi f(\hat H)\hat\pi = f(\hat\pi\hat H\hat\pi) + \mathcal{O}(\varepsilon^\infty)$ and $\hat\pi f(\hat h)\hat\pi =$

$\hat\pi f(\hat\pi\hat h\hat\pi)\hat\pi + \mathcal{O}(\varepsilon^2)$. Modulo $\mathcal{O}(\varepsilon^{2-n})$ we find

$$\begin{aligned}\mathrm{Tr}\left(\hat\pi f(\hat H)\,\hat a\right) &= \mathrm{Tr}\left(\hat\pi f(\hat H)\,\hat\pi\,\hat a\right) = \mathrm{Tr}\left(\hat\pi f(\hat\pi\hat H\hat\pi)\,\hat\pi\,\hat a\right)\\ &= \mathrm{Tr}\left(\hat\pi f(\hat\pi\hat h\hat\pi)\,\hat\pi\,\hat a\right) = \mathrm{Tr}\left(\hat\pi f(\hat h)\,\hat\pi\,\hat a\right).\end{aligned}$$

Next note that for scalar symbols the functional calculus for pseudo-differential operators implies that $f(\hat h) - \widehat{f(h)} = \mathcal{O}(\varepsilon^2)$. Hence with (6) we have up to $\mathcal{O}(\varepsilon^{2-n})$

$$\begin{aligned}\mathrm{Tr}\left(\hat\pi f(\hat H)\,\hat a\right) &= \int\frac{\mathrm{d}q\mathrm{d}p}{(2\pi\varepsilon)^n}\mathrm{tr}\left(f(h(q,p))\,(\pi\#a\#\pi)(q,p)\right)\\ &= \int\frac{\mathrm{d}q\mathrm{d}p}{(2\pi\varepsilon)^n} f(h(q,p))\;\mathrm{tr}\left((\pi\#a\#\pi)(q,p)\right).\end{aligned}$$

Using (2) and the fact that a is scalar, we have that the expansion of $A := \pi\#a\#\pi$ starts with $A_0 = \pi_0 a_0$ and

$$\begin{aligned}A_1 &= \pi_0 a_1\pi_0 + a_0\pi_1\pi_0 + a_0\pi_0\pi_1\\ &\quad -\tfrac{\mathrm{i}}{2}\pi_0\{a_0,\pi_0\} - \tfrac{\mathrm{i}}{2}\{\pi_0,a_0\}\pi_0 - \tfrac{\mathrm{i}}{2}a_0\{\pi_0,\pi_0\}\,.\end{aligned}$$

Taking the trace we get up to $\mathcal{O}(\varepsilon^2)$

$$\begin{aligned}\mathrm{tr}\,(\pi\#a\#\pi) &= a_0 + \varepsilon\left(\mathrm{tr}\,(\pi_0 A_1\pi_0) + \mathrm{tr}\left(\pi_0^\perp A_1\pi_0^\perp\right)\right)\\ &= a_0 + \varepsilon a_1 + \varepsilon 2a_0\mathrm{tr}\,(\pi_0\pi_1\pi_0)\\ &= a\left(1 + \mathrm{i}\varepsilon\,\mathrm{tr}\,(\pi_0\{\pi_0,\pi_0\})\right)\,,\end{aligned}$$

where we used (5), $\mathrm{tr}_{\mathcal{H}_\mathrm{f}}(\{\pi_0,\pi_0\}) = 0$ and (7).

2.2 Egorov theorem

Let ϕ^t_ε be the Hamiltonian flow of h with respect to the symplectic form ω_ε. Then the Heisenberg observable $A(t) := \mathrm{e}^{\mathrm{i}\hat H\frac{t}{\varepsilon}}\,\hat a\,\mathrm{e}^{-\mathrm{i}\hat H\frac{t}{\varepsilon}}$ can be approximated by transporting the symbol a of $A(0)$ along the classical flow ϕ^t_ε,

$$\hat\pi\left(A(t) - \widehat{a\circ\phi^t_\varepsilon}\right)\hat\pi = \mathcal{O}(\varepsilon^2)\,. \tag{9}$$

Proof: With $a(t) := a\circ\phi^t_\varepsilon$ we need to show that $\frac{\mathrm{d}}{\mathrm{d}t}\hat\pi\widehat{a(t)}\hat\pi = \frac{\mathrm{i}}{\varepsilon}[\hat\pi\hat H\hat\pi, \hat\pi\widehat{a(t)}\hat\pi] + \mathcal{O}(\varepsilon^2)$. Let $h_2 := \varepsilon^{-2}(\pi\#H\#\pi - \pi\#h\#\pi)$, then $\pi\#h_2\#\pi = h_2 + \mathcal{O}(\varepsilon^\infty)$ and hence its principal symbol satisfies $(h_2)_0 = \pi_0\,(h_2)_0\,\pi_0$. Thus

$$\tfrac{\mathrm{i}}{\varepsilon}\left[\hat\pi(\hat H - \hat h)\hat\pi, \hat\pi\widehat{a(t)}\hat\pi\right] = \mathrm{i}\varepsilon\left[\hat h_2, \widehat{\pi\# a(t)\#\pi}\right] + \mathcal{O}(\varepsilon^\infty)$$

is of order ε^2 and

$$\begin{aligned}\tfrac{\mathrm{i}}{\varepsilon}\left[\hat\pi\hat H\hat\pi, \hat\pi\widehat{a(t)}\hat\pi\right] &= \tfrac{\mathrm{i}}{\varepsilon}\left[\hat\pi\hat h\hat\pi, \hat\pi\widehat{a(t)}\hat\pi\right] + \mathcal{O}(\varepsilon^2)\\ &= \tfrac{\mathrm{i}}{\varepsilon}\hat\pi\left[\hat h, \widehat{a(t)}\right]\hat\pi \;-\; \tfrac{\mathrm{i}}{\varepsilon}\hat\pi\left(\hat h\hat\pi^\perp\widehat{a(t)} - \widehat{a(t)}\hat\pi^\perp\hat h\right)\hat\pi + \mathcal{O}(\varepsilon^2)\\ &= \tfrac{\mathrm{i}}{\varepsilon}\hat\pi\left[\hat h, \widehat{a(t)}\right]\hat\pi \;+\; \tfrac{\mathrm{i}}{\varepsilon}\hat\pi\left[[\hat h,\hat\pi]\,,\,[\widehat{a(t)},\hat\pi]\right]\hat\pi + \mathcal{O}(\varepsilon^2)\,.\end{aligned}$$

Since h and $a(t)$ are scalar, (3) implies

$$\begin{aligned}
\tfrac{\mathrm{i}}{\varepsilon}\left[\hat{h}, \widehat{a(t)}\right] &= \mathrm{Op}^{\mathrm{W}}(\{h, a(t)\}) + \mathcal{O}(\varepsilon^2) \\
\tfrac{\mathrm{i}}{\varepsilon}\left[\hat{h}, \hat{\pi}\right] &= \mathrm{Op}^{\mathrm{W}}(\{h, \pi_0\}) + \mathcal{O}(\varepsilon^2) \\
\tfrac{\mathrm{i}}{\varepsilon}\left[\widehat{a(t)}, \hat{\pi}\right] &= \mathrm{Op}^{\mathrm{W}}(\{a(t), \pi_0\}) + \mathcal{O}(\varepsilon^2)\,,
\end{aligned}$$

where $\mathrm{Op}^{\mathrm{W}}(\cdot) := \widehat{(\cdot)}$, and thus, again modulo $\mathcal{O}(\varepsilon^2)$,

$$\begin{aligned}
&\tfrac{\mathrm{i}}{\varepsilon}[\hat{\pi}\hat{H}\hat{\pi}, \hat{\pi}\widehat{a(t)}\hat{\pi}] = \\
&= \hat{\pi}\,\mathrm{Op}^{\mathrm{W}}\left(\{h, a(t)\} - \mathrm{i}\varepsilon[\{h, \pi_0\}, \{a(t), \pi_0\}]\right)\hat{\pi} \\
&= \hat{\pi}\,\mathrm{Op}^{\mathrm{W}}\left(\{h, a(t)\} - \mathrm{i}\varepsilon\mathrm{tr}\left(\pi_0[\{h, \pi_0\}, \{a(t), \pi_0\}]\right)\right)\hat{\pi}\,.
\end{aligned}$$

In order to compute $\partial_t a(t)$ recall that the Hamiltonian vector-field X_h with respect to ω_ε is $X_h^\alpha = -(\omega_\varepsilon)^{\alpha\beta}\partial_\beta h$ and thus by definition of $a(t)$ and Ω we have

$$\begin{aligned}
\frac{\partial a(t)}{\partial t} &= \begin{pmatrix} \partial_q a \\ \partial_p a \end{pmatrix}^T \begin{pmatrix} -\varepsilon\,\Omega^{pp} & E_n + \varepsilon\Omega^{pq} \\ -E_n + \varepsilon\Omega^{qp} & -\varepsilon\,\Omega^{qq} \end{pmatrix} \begin{pmatrix} \partial_q h \\ \partial_p h \end{pmatrix} \\
&= \{h, a(t)\} - \mathrm{i}\varepsilon\,\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(\pi_0[\{h, \pi_0\}, \{a(t), \pi_0\}]\right)\,.
\end{aligned}$$

2.3 Transport of Wigner functions

For $\psi \in \hat{\pi}\mathcal{H}$ we define the band Wigner function as

$$w_{\pi_0}^{\psi} := \left(1 - \mathrm{i}\varepsilon\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\left(\pi_0\{\pi_0, \pi_0\}\right)\right)\mathrm{tr}\,W^{\psi}\,,$$

where W^{ψ} is the standard Wigner function. Then $w_{\pi_0}^{\psi(t)} = w_{\pi_0}^{\psi} \circ \phi_\varepsilon^{-t} + \mathcal{O}(\varepsilon^2)$ in the sense that

$$\langle \psi(t),\, \hat{a}\,\psi(t)\rangle_{\mathcal{H}} = \int_{\mathbb{R}^{2n}} \mathrm{d}\lambda_\varepsilon\,(w_{\pi_0}^{\psi} \circ \phi_\varepsilon^{-t})(q,p)\,a(q,p) + \mathcal{O}(\varepsilon^2)$$

with $\psi(t) := \mathrm{e}^{-\mathrm{i}\hat{H}\frac{t}{\varepsilon}}\psi$ for all scalar bounded symbols a.

Proof: Using the invariance of λ_ε under the Hamiltonian flow ϕ_ε^t (Liouville's Theorem), one directly computes

$$\begin{aligned}
&\int_{\mathbb{R}^{2n}} \mathrm{d}\lambda_\varepsilon\,(w_{\pi_0}^{\psi} \circ \phi_\varepsilon^{-t})\,a = \int_{\mathbb{R}^{2n}} \mathrm{d}\lambda_\varepsilon\, w_{\pi_0}^{\psi}\,(a \circ \phi_\varepsilon^{t}) \\
&\quad = \langle \psi,\, \hat{A}(t)\,\psi\rangle_{\mathcal{H}} + \mathcal{O}(\varepsilon^2) = \langle \psi(t),\, \hat{a}\,\psi(t)\rangle_{\mathcal{H}} + \mathcal{O}(\varepsilon^2)\,.
\end{aligned}$$

2.4 Time-dependent Hamiltonians

It is straightforward to generalize the above statements to the case of a Hamiltonian $H(t,q,p)$ depending explicitly also on time. To this end one just adds the canonical pair (t,E) and applies the previous results to the symbol $K(t,q,E,p) = E + H(t,q,p)$. Its spectral projections $\pi_0(t,q,p)$ are

independent of E and the classical Hamilton function is $k(t,q,E,p) = E + h(t,q,p)$ with symplectic form $\omega = \omega_0 + \varepsilon\Omega(t,q,p)$, where h and Ω are computed from the instantaneous Hamiltonian $H(t,q,p)$ as before. The equations of motion are now

$$\begin{aligned} \dot q &= (1+\varepsilon\Omega^{pq})\partial_p h - \varepsilon\Omega^{pp}\partial_q h + \varepsilon\Omega^{pt} \\ \dot p &= (-1+\varepsilon\Omega^{qp})\partial_q h - \varepsilon\Omega^{qq}\partial_p h - \varepsilon\Omega^{qt}\,. \end{aligned} \tag{10}$$

On the side of quantum mechanics we have $(\mathrm{e}^{-\mathrm{i}\hat K\frac{t-t_0}{\varepsilon}}\psi)(t) = U^\varepsilon(t,t_0)\psi(t_0)$, where $U^\varepsilon(t,t_0)$ is the unitary propagator generated by $\hat H(t)$. The statement of the Egorov theorem becomes

$$\hat\pi(t_0)(A(t) - \widehat{a\circ\phi_\varepsilon^{t,t_0}})\hat\pi(t_0) = \mathcal{O}(\varepsilon^2)\,, \tag{11}$$

where $a\circ\phi_\varepsilon^{t,t_0}(q,p) = a(Q(t|t_0,q,p), P(t|t_0,q,p))$ and $Q(t|t_0,q,p), P(t|t_0,q,p)$ is the solution to (10) with initial data $Q(t_0|t_0,q,p) = q$ and $P(t_0|t_0,q,p) = p$.

2.5 The Piezo current in a magnetic field

As an illustration consider noninteracting electrons in a slowly deformed periodic crystal subject to a constant external magnetic field $\vec B_0 + \varepsilon\vec B$, where $\vec B_0$ has rational flux per unit cell. The crystal is modeled by a potential $V_\Gamma(t)$ periodic with respect to some lattice Γ. After a magnetic Bloch-Floquet transformation the Hamiltonian is the Weyl quantization $q\mapsto \mathrm{i}\varepsilon\nabla_p$, $p\mapsto p$, of the operator valued symbol

$$H_0(t,q,p) \;=\; \tfrac12(p - \mathrm{i}\nabla_y + \tfrac12 B_0 y + \tfrac12 Bq)^2 + V_\Gamma(y,t)$$

pointwise acting on $L^2(M_y)$, where M is the fundamental domain of a magnetic super-lattice $\tilde\Gamma$. It is convenient to write $B_{ij} = \epsilon_{ijk}(\vec B)_k$ for the following computations. Up to unitary equivalence $H_0(t,\kappa)$ is periodic in $\kappa = p + \frac12 Bq$ with respect to the dual lattice $\tilde\Gamma^*$ whose fundamental domain is the magnetic Brillouin zone $\mathbb{T}^*$. To each isolated magnetic Bloch band $e_0(t,\kappa)$ of H_0 with spectral projection $\pi_0(t,\kappa)$ we associate the classical system $h(t,\kappa) = e_0(t,\kappa) + \varepsilon M(t,\kappa)$. For $\Omega(\kappa)$ one finds $\Omega^{pt} = -\mathrm{i}\,\mathrm{tr}(\pi_0[\nabla\pi_0, \partial_t\pi_0])$, $\Omega^{pp}_{ij} = -\mathrm{i}\,\mathrm{tr}(\pi_0[\partial_{p_i}\pi_0, \partial_{p_j}\pi_0])$, $\Omega^{pq} = \frac12\Omega^{pp}B$, $\Omega^{qq} = -\frac14 B\Omega^{pp}B$. The classical equations (10) thus read

$$\dot q \;=\; \big(1+\varepsilon\Omega^{pp}(t,\kappa)B\big)\partial_\kappa h(t,\kappa) + \varepsilon\Omega^{pt}(t,\kappa), \quad \dot\kappa = B\dot q\,.$$

Note that all classical objects are $\tilde\Gamma^*$-periodic and hence the classical phase space is really $\mathbb{R}^3\times\mathbb{T}^*$. We can now approximate the current operator $J(t) := \frac1\varepsilon\frac{\mathrm d}{\mathrm dt}X(t)$ on the range of $\hat\pi(t_0)$ according to the Egorov theorem (11) and find that the current density when starting in the state $\rho(t_0) = f(\hat H(t_0))$ is

$$\begin{aligned} &\lim_{\Lambda\to\mathbb{R}^3}\tfrac{\varepsilon^3}{|\Lambda|}\mathrm{Re}\,\mathrm{Tr}\left(\hat\pi(t_0)f(\hat H(t_0))J(t)\,\chi_\Lambda(q)\right) \\ &\quad= \frac1\varepsilon\int_{\mathbb{T}^*}\frac{\mathrm d\lambda_\varepsilon(t)}{(2\pi)^3}\,\big(f(h(t_0))\circ\phi_\varepsilon^{t,t_0}\big)(\kappa)\;\dot q(t,\kappa) + \mathcal{O}(\varepsilon)\,. \end{aligned}$$

With $\mathrm d\lambda_\varepsilon(t) = (1+\varepsilon\vec\Omega(t)\cdot\vec B)\mathrm d\kappa$ and for a fully occupied band $f(h(t_0,\kappa))\equiv 1$ the leading term vanishes as can be seen by partial integration. The contribution to the Piezo current density from

this band is therefore

$$\begin{aligned} j(t) &= \int_{\mathbb{T}^*} \frac{\mathrm{d}\kappa}{(2\pi)^3} \left(\vec{B}\,\vec{\Omega}(t,\kappa)\cdot\nabla e_0(t,\kappa) + \Omega^{pt}(t,\kappa) \right) \\ &= \int_{\mathbb{T}^*} \frac{\mathrm{d}\kappa}{(2\pi)^3}\, \Omega^{pt}(t,\kappa)\,. \end{aligned}$$

The last equality follows again by partial integration and the fact that Ω^{pp} is a closed 2-form and thus the divergence of $\vec{\Omega}$ with $(\vec{\Omega})_i = \frac{1}{2}\epsilon_{ijk}\Omega^{pp}_{jk}$ vanishes. From this expression it is now straightforward to derive the King-Smith and Vanderbildt formula [8] for the orbital polarization, cf. [1, 9]. This shows that the orbital polarization is a geometric quantity that does not change under variations of the magnetic field as long as the Fermi energy lies in a gap between (magnetic) Bloch bands, see also [10] for systems with disorder. Note, however, that the result does not follow from the modified equations of motion (10) alone, but requires their correct application including the modified Liouville measure.

2.6 Concluding remarks

As mentioned before, the literature on adiabatic slow-fast systems is vast. Several groups [5, 1, 11, 9, 4] arrived independently and with different methods at equations more or less similar to (10). However, their precise connection to quantum mechanical expressions was not established before for (8), and only shown in a special case [11] for (9).

The most striking applications of the modified semiclassical model are due to Niu et al. [1]. They establish (10) as the equations of motion for the center of a Bloch wave packet. While it is natural to conclude from this also the formulas (8) and (11), they give, to our knowledge, no systematic derivation. In particular, they arrive at the correct Liouville measure λ_ε by looking for the invariant measure of (10) and then postulate (8). Moreover, in the case of nonzero magnetic field B_0 the magnetic Bloch bundle defined by $\pi_0(\kappa)$ over the torus $\mathbb{T}^*$ is not trivializable, which might present an obstruction to patching statements about localized wave packets together. Indeed, in [11] a rigorous derivation of (9) was given for Bloch electrons with $B_0 = 0$, which relies heavily, as also [2, 3, 4, 5] do, on the possibility to chose a global non-vanishing section of the Bloch bundle. The difficulties with generalizing the approach of [11] to magnetic Bloch bands led us to the new approach presented here.

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